M.Sc. (Part-II) (Chemistry) (CBCS Pattern) Semester - IV

# PSCHT13 - Paper-XIII : Spectroscopy

P. Pages : 3 **GUG/S/23/11448**

Time : Three Hours * 1 5 9 4 * Max. Marks : 80

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Notes : 1. All questions are compulsory.
2. All questions carry equal marks.

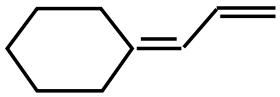
**1.** a) Discuss the different types of electronic transitions. Explain the effect of conjugation on electronic transition. **8**

b) Discuss the principle of photoelectron spectroscopy. Explain the photoelectron spectra of $N_2$ and HBr. **8**

**OR**

c) State and explain the Frank Condon principle. **4**

d) Discuss the Fiesher wood ward rules for dienes. Calculate the value of $\lambda_{max}$ for **4**



e) Give the applications of ESCA in structural determination. **4**

f) Explain the basic idea about Auger electron spectroscopy. **4**

**2.** a) Discuss the resonance condition in PMR spectroscopy. Explain the PMR spectra of $AX_2$ and AMX molecules with suitable example. **8**

b) What is Shielding and deshielding of protons? Explain the various factors affecting the chemical shift with suitable examples. **8**

**OR**

c) Define coupling constant. Discuss the variation of coupling constant with dihedral angle. **4**

d) Write a note on shift reagent. **4**

e) What is spin-spin interaction. Draw the PMR spectra of ethyl acetate. **4**

f) i) Give the Karplus equations. **4**
ii) Assign the structure on the basis of following data.
Molecular formula : $C_4H_8O_2$
PMR : $\delta 1.23$ (triplet, 3H)
$\delta 1.97$ (singlet, 3H)
$\delta 4.06$ (quartet, 2H)

**3.** a) Explain the following NMR spectroscopic techniques. **8**

i) COSY ii) DEPT

b) i) An organic compound having molecular formula $C_9H_{10}O_2$ exhibits the following spectral data **8**

IR : $1745cm^{-1}(s)$, $1225cm^{-1}(br,s)$, $749(s)$; $697cm^{-1}(s)$

UV : $\lambda_{max}$ at 268, 264, 262, 257 nm

$^1HNMR : \delta 1.96(3H,s)$; $5.00(2H,s)$; $7.22(5H,s)$

Deduce the structure of the compound

ii) An organic compound (Molecular weigh 108) is not acid, can be easily oxidized to a crystalline compound (m. pt. 122ºC). It gives the following spectral data

$UV : \lambda_{max}$ 255nm ($\varepsilon_{max} = 202$)

$IR : V_{max}^{cm^{-1}}$ $3402(s,br)$, $3065(w)$, $2888(m)$ $1499(w,sh)$, $1455(m)$

$^1HNMR :$ $\delta 3.90(singlet,1H)$

$\delta 4.60(singlet,2H)$

$\delta 7.26(singlet,5H)$

Deduce the structure of the compound

**OR**

c) Discuss the APT technique in brief. **4**

d) Explain the use of NMR in medical diagnosis. **4**

e) A compound with molecular formula $C_9H_5NO_4$ forms the following data in its infrared spectrum 3000-2500 (b), 2225 (m), 1715 (s), 1605, 1518(s),1344(s), $770cm^{-1}$ **4**

In NMR spectrum two bands are formed as

i) -1.1 $\tau$ (singlet, 1H)

ii) Unsymmetrical pattern 2.6-2.75 $\tau$ (4H) Determine the structural formula of the compound.

f) Write a note on: **4**

i) Quadrupole nuclei

ii) Quadrupole moment

**4.** a) Explain Bragg's condition. Discuss Debye Scherrer method for the x-rays analysis. **8**

b) Derive the Wierl equation of electron diffraction technique. Explain the technique scattering of neutron by solids and liquids. **8**

**OR**

c) Explain Laue method for the x-rays analysis. **4**

d) Explain how electron diffraction of gases is carried out. **4**

e) Distinguish the electron and neutron diffraction in brief. **4**

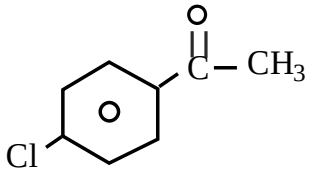
f) Determine atomic spacing in a NaCl crystal having cubic lattice; the density of NaCl is $2.16 \times 10^3 kg/m^3$ and the average masses of Na and Cl atoms are $3.82 \times 10^{-26} kg$ and $5.89 \times 10^{-26} kg$ respectively. **4**

**5.** a) Define with suitable examples. **2**

i) Chromophore

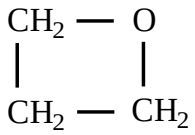
ii) Auxochrome

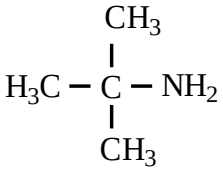
b) Calculate the absorption maximum for the following compound. **2**

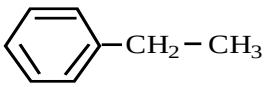


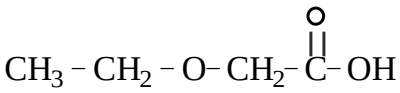
c) Compare $^{13}C-NMR$ spectroscopy with $^{1}H-NMR$ spectroscopy. **2**

d) How many $^{1}H-NMR$ signals are obtained in the following compounds. **2**

i) 

ii) 

iii) 

iv) 

e) Write a note on Nuclear overhouser effect. **2**

f) Give the advantages of FT-NMR. **2**

g) Calculate Miller indices of crystal planes which cut through the crystal axes at **2**

i) 2a, 3b, c

ii) 2a, -3b, -3c

h) Compare scattering intensity vs scattering angle. **2**

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